

TABLE OF CONTENTS

ACKNOWLEDGEMENTS.....	I
إهداء	II
ABSTRACT.....	III
ملخص.....	IV
TABLE OF CONTENTS	V
LIST OF FIGURES.....	VIII
LIST OF TABLES.....	XI
Chapter 1 PROBLEM STATEMENT.....	1
Chapter 2 INTRODUCTION.....	6
A) COMPUTATIONAL BACKGROUND.....	6
A.2.1 Schrödinger equation.....	6
A.2.2 Schrödinger equation for hydrogen atom.....	7
A.2.3 Schrödinger equation for helium atom.....	10
A.2.4 Schrödinger equation for molecules.....	11
A.2.5 Approximation methods.....	13
A.2.5.1 Variation method.....	14
A.2.5.2 Perturbation method.....	18
A.2.6 Basis set.....	20
A.2.6.1 Functional form.....	21
A.2.6.2 Contracted Gaussian Functions and minimal basis set.....	23
A.2.6.3 Multiple Zeta (ζ), and split valence.....	25
A.2.6.4 Polarization functions.....	28
A.2.6.5 Diffused functions.....	29
A.2.6.6 Effective core potential (ECP).....	30
A.2.7 Electronic Structure calculation Methods.....	31
A.2.7.1 Ab-initio methods.....	32

A.2.7.1.1 Hartree-Fock self-consistent field method(HF-SCF).....	32
A.2.7.1.2 Configuration Interaction (CI).....	40
A.2.7.1.3 Moller-Plesset Perturbation Theory.....	41
A.2.7.2 Semiempirical method.....	41
A.2.7.3 Density Functional Theory (DFT).....	42
 B) CHEMICAL BACKGROUND.....	48
B.2.1 Metal Carbonyl complexes.....	48
B.2.2 Trans effect.....	51
B.2.3 Metal-alkene complexes.....	53
B.2.4 Metal-Alkyne complexes.....	55
 Chapter 3 METHODS, RESULTS, AND DISCUSSION.....	60
3.1 Methods.....	60
3.2 Results and discussion.....	61
3.2.1 Molecular Geometry Analysis.....	61
3.2.1.1 Pentacarbonyl(3,3-diethyl-5-methoxycarbonyl-3H-pyrazol- N2)chromium (0).....	61
3.2.1.2 Methyl prop-2-ynoate.....	68
3.2.1.3 η^2 - Methyl prop-2-ynoate (pentacarbonyl)-chromium.....	70
3.2.1.4 3-Diazopentane.....	73
3.2.1.5 3,3-Diethyl-5-methoxycarbonyl-3H-pyrazole.....	75
3.2.1.6 Pentacarbonyl (3,3-diethyl-5-methoxycarbonyl-3H-pyrazol-C2)chromium (0).....	77
3.2.2 Thermochemical analysis.....	83
3.2.2.1 Path (a) analysis.....	84
3.2.2.1.1 The addition of 3-diazopentane to η^2 -methyl prop-2-ynoate(pentacarbonyl)chromium to form Pentacarbonyl(3,3-diethyl-5-methoxycarbonyl-3H-pyrazol-C2)chromium(0).....	84
3.2.2.1.2 Rearrangement of Pentacarbonyl(3,3-diethyl-5-methoxycarbonyl-3H-pyrazol-C2)chromium(0) to give pentacarbonyl(3,3-diethyl-5-methoxycarbonyl-3H-pyrazol-N2)chromium (0).....	86
3.2.2.2 Path (b) analysis.....	88
3.2.2.2.1 The disociation of the η^2 -Methyl prop-2-ynoate(pentacarbonyl)chromium	88
3.2.2.2.2 The cycloadditon of the alkyne to the 3-Diazopentane.....	88
3.2.2.2.3 The Cr-N bond brakeage in pentacarbonyl (3,3-diethyl-5-methoxycarbonyl-3H-pyrazol-N2)chromium(0).....	90

Chapter 4 CONCLUSIONS AND RECOMENDATION	91
REFERENCES.....	94
APPENDIX.....	102
Appendix References.....	121